ON TAKING ACCOUNT OF THE CRYSTAL-LATTICE FIELD IN STUDYING THE INTERACTION OF ELECTRONS WITH A RANDOMLY DISTRIBUTED IMPURITY

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Abstract

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V. K. PETERSON

ON TAKING ACCOUNT OF THE CRYSTAL-LATTICE FIELD IN STUDYING THE INTERACTION OF ELECTRONS WITH A RANDOMLY DISTRIBUTED IMPURITY

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In studying the interaction of conduction electrons with a randomly distributed impurity, the presence of the crystal lattice is usually taken into account by the effective-mass method [1–4]. In the present work, perturbation theory is developed for the Green' s function, using as the zeroth approximation the Green' s function of quasiparticles located in the periodic field of the crystal. The behavior of the mass operator near the Fermi surface is investigated in the one-zone approximation.

Let us consider a quantum-mechanical system consisting of quasiparticles located in an external field. The external field consists of a periodic part (the field of the crystal), which is taken into account in the unperturbed Hamiltonian, and of the field created by N "randomly" situated impurity particles. We denote the latter part of the external field by

$$W_A(x) = \sum_{x_a \in A} W(|x - x_a|)$$

(A is the totality of the coordinates of all impurity particles).

Introduce the causal Green' s function of the system with impurity, $G_A(x, y)$. Passing to the $n, \mathbf{k}, E$-representation, we obtain

$$G_A(x, y) = \int \frac{dE}{2\pi} \frac{1}{V^2} \sum_{n,\mathbf{k},l,\mathbf{k}_1} G_A(n, \mathbf{k}; l, \mathbf{k}_1; E)\, \psi_{n\mathbf{k}}(x) \psi^*_{l\mathbf{k}1}(y) e^{-iE(x_0 - y_0)}$$

(n is the band index, $\hbar\mathbf{k}$ is the quasimomentum, $\psi_{n\mathbf{k}}$ is an eigenfunction of the equation taking account only of the periodic field, V is the volume of the system).

Perturbation theory leads to the equation

$$G_A(n,\mathbf{k};l,\mathbf{k}_1;E) = G_0(n,\mathbf{k};E)\delta_{nl}\cdot V\delta_{\mathbf{kk}_1} - G_0(n,\mathbf{k};E)\frac{1}{V}\sum_{m,\mathbf{k}2} W_{Anm}^{\mathbf{kk}_2} G_A(m,\mathbf{k}_2;l,\mathbf{k}_1;E),$$

where $G_0(n,\mathbf{k};E)$ is the Green' s function of the system without impurity, and

$$W_{Anm}^{\mathbf{kk}_2} = \int d^3z\, \psi_{n\mathbf{k}}^*(z) W_A(z) \psi_{l\mathbf{k}2}(z).$$

In what follows the averaged Green' s function is considered. By averaging over different positions of the impurity particle is meant the procedure

$$\langle f\rangle = \int_\Omega \frac{d^3\xi}{\Omega}\,\varphi(\vec{\xi})\,\frac{1}{N_\Omega}\sum_{\mathbf{c}} f(\mathbf{c}+\vec{\xi}).$$

Here the impurity coordinates are represented as $\mathbf{c}+\vec{\xi}$ ($\mathbf{c}$ is a vector of the direct lattice of the crystal; $\vec{\xi}$ is the vector determining the position of the impurity particle inside the cell specified by the vector $\mathbf{c}$, i.e. $\vec{\xi}\in\Omega$, where Ω is the volume of the cell); f is the function being averaged; N_Ω is the number of crystal cells; $\varphi(\vec{\xi})$ is some function taking into account the probability distribution of the impurity inside the cell.

Averaging over all positions of N impurities is regarded as averaging over all positions of each impurity particle independently of the others.

Introduce the averaged Green' s function

$$G(n,\mathbf{k};l,\mathbf{k}_1;E) = \langle G_A(n,\mathbf{k};l,\mathbf{k}_1;E)\rangle =$$

$$= G_0(n,\mathbf{k};E)\delta_{nl} - G_0(n,\mathbf{k};E)\frac{1}{V^2}\sum_{m\mathbf{k}2}\langle W_{Anm}^{\mathbf{kk}_2} G_A(m,\mathbf{k}_2;l,\mathbf{k}_1;E)\rangle.$$

Since $\langle W_A\rangle = N\langle W(|\mathbf{z}-\mathbf{x}|)\rangle$ is a periodic function, without restricting generality we shall assume that

$$\langle W_A\rangle = 0, \qquad \text{i.e. } G^{(1)} = 0.$$

In the second order we obtain

$$G^{(2)}(n,\mathbf{k};l,\mathbf{k}_1;E) =$$

$$= \frac{N}{V}G_0(n,\mathbf{k};E)\frac{1}{V}\sum_{m\mathbf{k}2}\int_\Omega d^3\xi\,\varphi(\xi)\,W_{nm}^{\mathbf{kk}_2}(\xi)G_0(m,\mathbf{k}_2;E)W_{ml}^{\mathbf{k}_2\mathbf{k}}(\xi)G_0(l,\mathbf{k};E)\,V\delta_{\mathbf{kk}_1};$$

$\delta_{\mathbf{k}\mathbf{k}_1}$ expresses the law of conservation of quasimomentum. Since $V\delta_{\mathbf{k}\mathbf{k}_1}$ occurs in all orders, one may put

$$G(n,\mathbf{k};l,\mathbf{k}_1;E) = G(n,l;\mathbf{k};E)V\delta_{\mathbf{k}\mathbf{k}_1}.$$

For $G(n,l;\mathbf{k};E)$ we obtain, in the diagram representation, the following series:

[diagrammatic series of Green' s-function lines with one, two, and higher dashed impurity contractions]

In the fifth order for the Green' s function we obtain 11 diagrams, and in the sixth order, 41 diagrams.

To each chain of dashed lines there corresponds an operation of averaging over impurity positions inside the cell and a factor N/V. All sums of wave vectors entering the conservation laws are reduced. Otherwise the rules for constructing the diagram contributions are the usual ones.

Define in the usual way the mass operator M as the collection of diagrams without external lines which cannot be split into two parts by cutting only one solid line.

The Green' s function and the mass operator are related by the equation

$$G(n,l;\mathbf{k};E) = G_0(n,\mathbf{k};E)\delta_{nl} - G_0(n,\mathbf{k};E)\sum_h M(n,h;\mathbf{k};E)G(h,l;\mathbf{k};E).$$

Next introduce the interaction kernel (generalized vertex) D by means of the equation

$$D_{nh}^{\mathbf{k}\mathbf{k}_1}(\xi;E) = W_{nh}^{\mathbf{k}\mathbf{k}_1}(\xi) - \frac{1}{V}\sum_{s,r,\mathbf{k}2} D_{ns}^{\mathbf{k}\mathbf{k}_2}(\xi;E)G(s,r;\mathbf{k}_2;E)W_{rh}^{\mathbf{k}_2\mathbf{k}_1}(\xi).$$

Using D, the series for M can be represented in the form

[diagrammatic expression for M as a sum of a one-vertex term, a higher vertex chain, and $\cdots$] (1)

For the purpose of further contracting series (1), introduce the vertex part $-\Gamma$ by means of the following collection of graphs

[diagrammatic series defining Γ, with multiple solid-line chains and dashed contractions] (2)

Using (2), we obtain an expression for $-M$

(M) = [[diagram: one closed line with one impurity vertex]]

We obtain the expression for the interaction energy of quasiparticles with the impurity in the usual way, replacing $W_A \to gW_A$. After averaging, for $\Delta E(N) = \langle E_A \rangle - E_0$ we shall have ($\varepsilon \to +0$):

$$\Delta E(N) = -V \int_{-\infty}^{+\infty} \frac{dE}{2\pi i} e^{i\varepsilon E} \int_0^1 \frac{dg}{g} \frac{1}{V} \sum_{nmk} M(n, m; \mathbf{k}; E \mid g) G(m, n; \mathbf{k}; E \mid g). \tag{3}$$

Expanding (3) in orders, we obtain a series for $\Delta E(N)$

$\Delta E(N) =$ [[diagram: closed line with one interaction]]+[[diagram: closed triangle-like diagram]]+[[diagram: c

In the fifth order $\Delta E(N)$ has 3 diagrams, in the sixth 12. The rules for forming the contributions of vacuum (closed) diagrams are supplemented by the operation

$$V \frac{s}{n} \int_{-\infty}^{+\infty} \frac{dE}{2\pi i} e^{i\varepsilon E} \dots,$$

where n is the order of the diagram, and s is the structural multiplier, equal to the number of topologically distinct solid lines in the diagram.

Near the Fermi surface, some diagrams of the series M give divergent contributions. These divergences are connected with the shift of the singular point of the mass operator (5). To study the behavior of the mass operator in this region it is necessary to perform a partial summation. Since the divergences arise only in the unfilled band, in what follows the one-band approximation is considered. In this case the vertex connecting solid lines with momenta $\hbar\mathbf{k}$ and $\hbar(\mathbf{k} + \mathbf{q})$ corresponds to the Fourier component $Q(q)$:

$$Q(q) = \int_{V \to \infty} d^3u \, W(u) e^{-i\mathbf{qu}} = \frac{4\pi}{q} \int_0^\infty uW(u) \sin(qu) \, du.$$

Assuming that $Q(0) \neq \infty$, we introduce the effective interaction radius α^{-1} by means of

$$\frac{4\pi e^2}{\varepsilon_0 \alpha^2} = Q(0) = 4\pi \int_0^\infty u^2 W(u) \, du.$$

In what follows we shall deal with the dimensionless quantities $G, M, E, n = N/V\alpha^3$, $\mathbf{x} = \mathbf{q}/\alpha$, $f(x) = Q(\alpha x)/Q(0)$, and with the dimensionless interaction constant $\beta = 8\pi/a_B\alpha$ ($a_B = \hbar^2\varepsilon_0/me^2$), taking α^{-1} as the unit of length and $\hbar^2\alpha^2/2m$ as the unit of energy.

Concerning the function $f(x)$ we shall assume that: 1) $|f(x)| \leqslant 1$, for $x \leqslant 1$; 2) $|f(x)| \leqslant 1/x^2$ for $x > 1$. In addition, we put $f(x) = f_1(x^2)$ and shall assume that: 3) $|\partial f_1(u)/\partial u| \leqslant 1$, for $u \leqslant 1$, and 4) $|\partial f_1(u)/\partial u| \leqslant 1/u^2$ for $u > 1$ $(u = x^2)$.

For the Debye screening law $f(x) = (1 + x^2)^{-1}$.

For $|E - x_F^2| \sim \varepsilon$, allowance for the most divergent diagrams leads to the series

$$M_1(x^2; E) = \underset{\sim n\beta^2}{[[\text{diagram: one arc}]]} + \underset{\sim n^2\beta^4\,\frac{1}{\varepsilon}}{[[\text{diagram: two nested arcs}]]} + \underset{\sim n^3\beta^6\,\frac{1}{\varepsilon^2}}{[[\text{diagram: one large arc over two small arcs}]]} \tag{4}$$

Divergences are associated with a change in the sign of the imaginary increment $\pm i\varepsilon$ and arise in diagrams with self-energy insertions.

The series (4) converges only for $n\beta^\rho \dfrac{1}{\varepsilon} < 1$. Summation of the series leads to the equation [6] $\left(\lambda = \pi n\beta^2 \dfrac{1}{(2\pi)^3}\right)$:

$$-M_1(x^2; E) = n\beta^2 \int \frac{d^3z}{(2\pi)^3} \frac{f^2(|\mathbf{x} - \mathbf{z}|)}{z^2 - E + M_1(z^2; E)} =$$

$$= \frac{\lambda}{x} \int_0^\infty dy\, f^2(y)\, y \int_{(x-y)^2}^{(x+y)^2} \frac{du}{u - E + M_1(u; E)}. \tag{5}$$

Let us introduce the Fermi energy

$$E_F = \left\langle \frac{\partial}{\partial N} E_A(N) \right\rangle = x_F^2 + \operatorname{Re} M(x_F^2; E_F). \tag{6}$$

Solving equation (5) asymptotically as $\lambda \to 0$, using (6) and the condition imposed on the causal Green' s function ($\operatorname{Im} M$ changes sign at $E = E_F$), we obtain:

$$\operatorname{Re} M_1(x^2; E) = -\frac{\lambda}{x} \int_0^\infty dy\, f^2(y)\, y \ln \left| \frac{(x+y)^2 - E}{(x-y)^2 - E} \right|,$$

$$\operatorname{Im} M_1(x^2; E) = \operatorname{sign}(E_F - E) \frac{\lambda\pi}{x} \int_{|x-\sqrt{E}|}^{x+\sqrt{E}} dy\, f^2(y)\, y.$$

$\operatorname{Re} M_1$ does not differ from $\operatorname{Re} M^{(2)}$, which is obtained from the second-order diagram; however, $\operatorname{Im} M_1$, in contrast to $\operatorname{Im} M^{(2)}$, changes sign not at $E = x_F^2$, but at $E = E_F$.

$\operatorname{Im} M_1$ as $E \to E_F$ does not tend to zero, i.e., the transition to the region of negative values upon crossing the Fermi surface occurs discontinuously. This feature of the behavior of $\operatorname{Im} M$ is retained also in subsequent orders of the rearranged perturbation theory and is a characteristic feature of the model under investigation.

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Moscow State University
named after M. V. Lomonosov

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Note: Figure translations are in progress. See original paper for figures.